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DERIVATION OF A GENERALIZED VON NEUMANN PSEUDO-VISCOSITY WITH DIRECTIONAL PROPERTIES

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Gerald T. Richards
Captain, U. S. Army

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ABSTRACT

An absolute scalar pseudo-viscosity (" q ") expression for handling shocks automatically in numerical calculations of three-dimensional fluid dynamics problems is derived. The expression is a generalization of that derived by von Neumann and Richtmyer in the sense that the expressions are identical for a plane shock wave. The basic assumption made is that a shock will be formed in a material when there is compression in the direction of acceleration; this assumption seems "reasonable" physically, since this condition indicates that a grid established about a point with such compression will collapse, i.e., the "rear" of the grid will overtake the "front."

The expression " q " is derived for a generalized curvilinear coordinate space and the expression is given for the three commonly used coordinate systems. The expression is also written for the plane rectangular case and the cylindrical case with no angular motion to be used in connection with the HEMP code.

INTRODUCTION

The use of a pseudo-viscosity to handle shocks automatically in numerical calculations of fluid dynamics problems is well known.¹ The first programs written were for the solutions of problems in one space dimension for which the pseudo-viscosity (" q ") devised by von Neumann and Richtmyer was derived. However, the expression for " q " in this one-dimensional geometry did not carry over directly into more than one dimension. One of the expressions

¹ von Neumann and R. D. Richtmyer, "Finite Difference Methods for Initial-value Problems" (Interscience Publishers Inc., New York, 1957) p. 205 ff.

used for a two dimensional program involves the time rate of change of relative volume divided by relative volume $(\dot{V}/V)^2$ which in one dimension is equivalent to the gradient of the velocity used by von Neumann and Richtmyer. However, in a cylindrical or spherical implosion, the term \dot{V}/V will become negative (forming a shock) simply because the mass is being forced into the center even though the rear of a particular grid is not overtaking the front of that grid. The derivation given here overcomes this difficulty and is, in fact, a straight forward generalization of the expression devised by von Neumann and Richtmyer in the sense that the "q" was required to indicate that compression is present in the direction of acceleration, to turn itself on when this condition develops, and to give the same expression when a plane shock passes through a "one dimensional material." The expression derived differs from theirs in that it is formed from vector quantities in three space dimensions and the plane shock is not required to be parallel to one of the coordinate planes in order for the "q" to work. The basic assumption made is that a shock will be formed when there is compression in the direction of the acceleration. The "q" so derived is an absolute scalar formed from the product of an absolute second-order tensor and two vectors and could be used even in three dimensions.

THE DERIVATION OF A GENERALIZED VON NEUMANN SCALAR "q" WITH DIRECTIONAL PROPERTIES³

Consider a body that, under some unspecified force system, is undergoing motion which will, in general, include rigid body translation and rotation as well as deformation (Fig. 1). Let:

X^K ($K = 1, 2, 3$) refer to the coordinates of a point in the body in a fixed, Lagrange, generalized coordinate system.

x^k ($k = 1, 2, 3$) refer to the coordinates of the same point in a moving, Eulerian, generalized coordinate system.

Z^K ($K = 1, 2, 3$) be a fixed rectangular coordinate system.

z^k ($k = 1, 2, 3$) be a moving rectangular coordinate system.

²Mark L. Wilkins, "Calculation of Elastic-Plastic Flow," Lawrence Radiation Laboratory (Livermore) UCRL-7322 (1963).

³The derivation and notation are taken largely from Chapters 1 and 2 of Nonlinear Theory of Continuous Media by A. Cemal Eringen (McGraw-Hill Book Co., Inc., New York, 1962).

- $\underline{\underline{P}}$ be the position vector to (X^1, X^2, X^3) in the Z^K system.
 $\underline{\underline{p}}$ be the position vector to (x^1, x^2, x^3) in the z^k system.
 $\underline{\underline{b}}$ be the vector that represents the rigid translation of the body.
 $\underline{\underline{G}}_K$ be a base vector in the direction of X^K from (X^1, X^2, X^3) .
 $\underline{\underline{g}}_k$ be a base vector in the direction of x^k from (x^1, x^2, x^3) .
 t be the time.

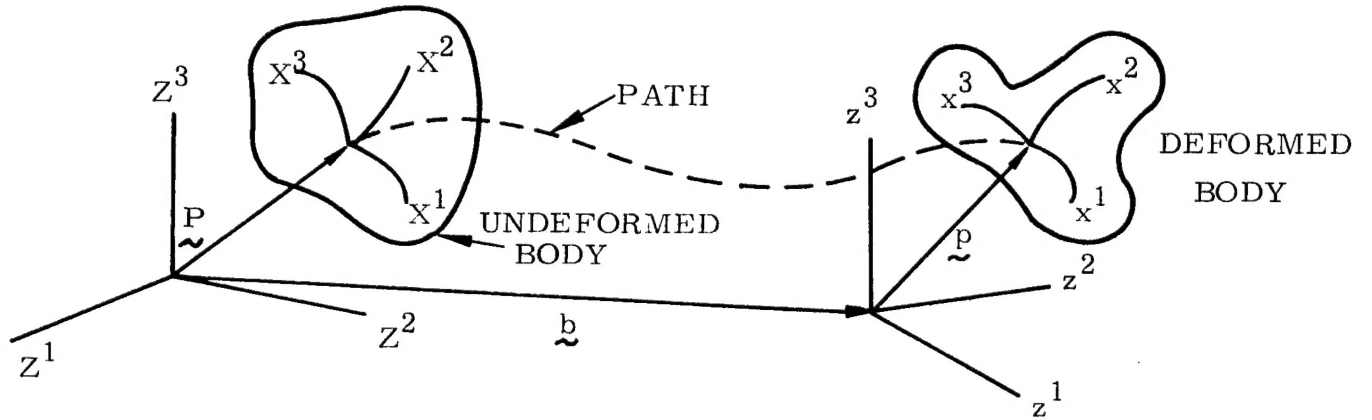


Fig. 1

Then the motion at any time is expressed as:

$$X^K = X^K(x^1, x^2, x^3, t) \text{ or } x^k = x^k(X^1, X^2, X^3, t). \quad (1)$$

From Eq. (1) we can determine the path taken by a point in the undeformed body at (X^1, X^2, X^3) as a function of x^k and t and conversely, we can determine the path taken to (x^1, x^2, x^3) as a function of X^K and t (in this treatment the inverse of $X^K(x^1, x^2, x^3, t)$ is assumed to exist). In other words, given a point in the undeformed body, we can determine where it goes and given a point in the deformed body we can determine where it came from in the undeformed body.

Consider a differential change in $\underline{\underline{P}}$ in the generalized Lagrange coordinate system. This differential is expressed by:

$$d\underline{\underline{P}} = \underline{\underline{G}}_K dX^K = \underline{\underline{G}}_1 dX^1 + \underline{\underline{G}}_2 dX^2 + \underline{\underline{G}}_3 dX^3 \quad (2)$$

and the square of the magnitude of this vector is:

$$dS^2 = d\underline{\underline{P}} \cdot d\underline{\underline{P}} = G_{KL} dX^K dX^L, \quad (3)$$

where $G_{KL} = \underline{\underline{G}}_K \cdot \underline{\underline{G}}_L$ is the metric tensor for the X^K system of coordinates.

Similarly, for the Eulerian coordinate system one obtains:

$$d\underset{\sim}{p} = \underset{\sim}{g}_k dx^k \quad (4)$$

along with its magnitude squared:

$$ds^2 = d\underset{\sim}{p} \cdot d\underset{\sim}{p} = g_{k\ell} dx^k dx^\ell, \quad (5)$$

where $g_{k\ell} = \underset{\sim}{g}_k \cdot \underset{\sim}{g}_\ell$ is the metric tensor for the x^k coordinate system.

The quantities dS^2 and ds^2 can be interpreted as the square of an element of arc length before deformation and after deformation respectively. It is, therefore, possible to obtain a measure of the deformation produced by the motion by calculating $ds^2 - dS^2$.

The material or substantial derivative is a time derivative with the Lagrange coordinate X^K held constant. It is denoted by D/Dt and it can be shown that (see Appendix A):

$$\frac{D}{Dt} (ds^2) = 2 d_{k\ell} dx^k dx^\ell, \quad (6)$$

where $d_{k\ell} \equiv \frac{1}{2} (v_{k;\ell} + v_{\ell;k})$ is the symmetric part of the velocity gradient, is called the deformation rate tensor, and is an absolute second-order tensor. $v_{k;\ell}$ is the covariant partial derivative of v_k (see Appendix A, Eq. (A.1)).

From (6) we see that:

$$\frac{1}{ds} \frac{D}{Dt} (ds^2) = \frac{2}{ds} \frac{D}{Dt} (ds) = 2 d_{k\ell} \frac{dx^k}{ds} \frac{dx^\ell}{ds}$$

or

$$\frac{1}{ds} \frac{D}{Dt} (ds) = d_{k\ell} n^k n^\ell = d_{(\underset{\sim}{n})} \quad (7)$$

where $dx^k/ds = n^k$ is the unit vector along ds , and $d_{(\underset{\sim}{n})}$ is called the rate of stretching or rate of deformation.

Since dS is a function of X^K only:

$$\frac{D}{Dt} (ds - dS) = \frac{D}{Dt} (ds) \quad (8)$$

so we see that (7) is a measure of the rate of change of deformation with respect to time divided by the current length of an element in the direction $\underset{\sim}{n}$. Hence, (7) can be used to determine whether there is tension or compression in the direction $\underset{\sim}{n}$, where $\underset{\sim}{n}$ is an arbitrary unit vector. In other words, given an arbitrary direction and a point $p(x^1, x^2, x^3)$ in a deforming

body, (7) can be used to determine whether an element of length in that direction is lengthening or shortening with time at a selected time t .

Consider a body in motion, select a point in this body at $p(x^1, x^2, x^3)$. One of the characteristics of a von Neumann "q" is that it is activated if the motion of $p(x^1, x^2, x^3)$ is a deceleration, i.e., the grid is collapsing in the direction of acceleration. It is clear that if the vector n^k in (7) is a unit vector in the direction of the acceleration vector, then (7) will be able to measure this effect, i.e., if

$$d_{(n)} = \frac{1}{ds} \frac{D}{Dt} (ds) < 0,$$

then, with $n^k = A^k / |\underline{A}|$, the grid is collapsing in the direction of motion, where \underline{A} is the acceleration vector.

It is important to note here that $d_{(n)}$ is completely independent of the coordinate system that is used to express $d_{k\ell}$ and n^k . This is easily seen from the method of derivation since the element $ds^2 = d\underline{p} \cdot d\underline{p}$ is a scalar derived from the scalar product of two vectors. This can also be seen from (7) as follows: Since $d_{k\ell}$ is an absolute covariant tensor of second order, a transformation of coordinates from x^k to \bar{x}^k through

$$d\bar{x}^k = \frac{\partial \bar{x}^k}{\partial x^\ell} dx^\ell$$

results in a transformation of $d_{k\ell}$ to $d'_{k\ell}$ by

$$d'_{k\ell} = d_{mn} \frac{\partial x^m}{\partial \bar{x}^k} \frac{\partial x^n}{\partial \bar{x}^\ell},$$

by definition. The contravariant vector n^k will transform to \bar{n}^k by

$$\bar{n}^k = n^m \frac{\partial \bar{x}^k}{\partial x^m}.$$

We now form, using these,

$$d'_{k\ell} \bar{n}^k \bar{n}^\ell = d_{mn} \frac{\partial x^m}{\partial \bar{x}^k} \frac{\partial x^n}{\partial \bar{x}^\ell} n^r \frac{\partial \bar{x}^k}{\partial x^r} n^p \frac{\partial \bar{x}^\ell}{\partial x^p}$$

$$d'_{k\ell} \bar{n}^k \bar{n}^\ell = d_{mn} \frac{\partial x^m}{\partial \bar{x}^k} \frac{\partial \bar{x}^k}{\partial x^r} \frac{\partial x^n}{\partial \bar{x}^\ell} \frac{\partial \bar{x}^\ell}{\partial x^p} n^r n^p$$

$$d'_{k\ell} \bar{n}^k \bar{n}^\ell = d_{mn} \delta_r^m \delta_p^n n^r n^p$$

where

$$\delta_{ij}^i = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \equiv \text{Kronecker delta}$$

or

$$d'_{k\ell} \bar{n}^k \bar{n}^\ell = d_{mn} n^m n^n.$$

This invariance with respect to an arbitrary coordinate system is the chief property of interest in this expression. In the HEMP² code the "Q" is based on \dot{V}/V , where V is the relative volume. In a spherical or cylindrical implosion the expression \dot{V}/V becomes negative simply because the mass is being crowded in to a smaller and smaller space while in the direction of acceleration, the front surface of the grid (the one toward the center) is moving faster than the rear surface. The quantity $d_{(\underline{n})}$ would indicate this clearly, if \underline{n} were a vector in the direction of the acceleration vector.

If we consider a shock moving through a material at rest and making an angle with the coordinate system x^k , i.e., not along any of x^1, x^2, x^3 , then a coordinate system can be selected such that one coordinate α lies along the acceleration vector and the other two coordinates (β, γ) are normal to α .

Then

$$n^1 = 1, \quad n^2 = 0, \quad n^3 = 0$$

and

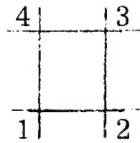
$$d_{(\underline{n})} = d_{(\alpha)} = d_{\alpha\alpha} = \frac{1}{2} (v_{\alpha;\alpha} + v_{\alpha;\alpha}) = \frac{\partial v_\alpha}{\partial \alpha},$$

where v_α is the velocity in the α direction and, in this case, is in the direction of the shock. In other words, $d_{(\underline{n})} = d_{(\alpha)}$ is the partial derivative of the velocity in the direction of the shock with respect to the space coordinate in the direction of the shock. We see, therefore, that this is the same expression used by von Neumann and Richtmyer¹ in the "activating" part of the artificial viscosity and all that has been done here is to express it in a generalized form.

The sticky part of the problem involves the selection of the characteristic length to be used to multiply the activation term and spread the shock over the same number of zones in the numerical solution. von Neumann and Richtmyer used ΔX , the Lagrange grid size in the direction of the shock (see Ref. 1, p. 215 ff). In this case our grid is established in the system X^K , is allowed to

deform in the system x^k and is not in general in the direction of the shock. Conceptually a grid length ΔA could be established in the shock direction, corresponding to α above, and this could be transformed to the X^K coordinate system, but in practice this cannot be done since the grids are already established in the X^K system. The approach taken here was to use the established grid to determine a representative length in the direction of the acceleration.

Two lengths were tried (ΔS_1 and ΔS_2). ΔS_1 was formed as the arithmetic average of the projections of the two grid diagonals in a two-dimensional grid on the acceleration direction. ΔS_2 was formed as the square root of the sum (or average) of the geometric averages of the separate components of the diagonals projected on the acceleration direction. If the figure below represents the grid at time step t and the quantities n^1 and n^2 are understood to be calculated at the midpoint of the grid at time step t , then the expressions used are:



GRID

$$\Delta S_1 = \frac{|(X_3 - X_1)n^1 + (Y_3 - Y_1)n^2| + |(X_2 - X_4)n^1 + (Y_2 - Y_4)n^2|}{2}$$

$$\Delta S_2 = \left[(n^1)^2 |X_3 - X_1| |X_2 - X_4| + (n^2)^2 |Y_3 - Y_1| |Y_2 - Y_4| \right]^{1/2}$$

where $|B|$ is the absolute value or magnitude of B , and where

$$n^i = \frac{\frac{1}{\rho} t_{;j}^{ji} + f^i}{\left| \frac{1}{\rho} t_{;j}^{ji} + f^i \right|}, \quad i, j = 1, 2$$

are the general expressions for the direction cosines in the acceleration direction (see Ref. 3, p. 104). (Here t^{ij} is the stress tensor, f^i the body force per unit mass, and ρ the mass density.) The factors of $1/2$ needed in the averages are to be embodied in a multiplicative constant.

In the limit of a shock in one dimension, let $\dot{Y} = 0$, then:

$$\Delta S_1 = \frac{|X_3 - X_1| + |X_2 - X_4|}{2}$$

$$\Delta S_2 = \left[|X_3 - X_1| |X_2 - X_4| \right]^{1/2}.$$

So the grid size in the non-shock direction is not considered in the one-dimensional shock as would be desired. Further, if the grid is square, then $|X_3 - X_1| = |X_2 - X_4|$ and $\Delta S_1 = \Delta S_2 = \Delta X$ which is the factor used by von Neumann and Richtmyer.

In the problems worked using this "q," there was no obvious difference between the two ΔS 's. Some experimentation would be required in order to make a selection.

The HEMP code is a two-dimensional code with plane or cylindrically symmetric geometry and the expression for $d_{(\tilde{n})}$ is (see Appendix B):

$$d_{(\tilde{n})} = \frac{\partial \dot{X}}{\partial X} (n^1)^2 + \frac{\partial \dot{Y}}{\partial Y} (n^2)^2 + \left(\frac{\partial \dot{X}}{\partial Y} + \frac{\partial \dot{Y}}{\partial X} \right) n^1 n^2$$

where Y is either the radial direction or the other rectangular direction. In this code we have used both a linear and a quadratic "q" as follows:

Linear:

$$q = 0 \text{ if } d_{(\tilde{n})} \geq 0$$

$$q = -C_L \frac{\rho_0^a}{V} d_{(\tilde{n})} \Delta S \text{ if } d_{(\tilde{n})} < 0$$

Quadratic:

$$q = 0 \text{ if } d_{(\tilde{n})} \geq 0$$

$$q = C_O^2 \frac{\rho_0^0}{V} \left(d_{(\tilde{n})} \right)^2 (\Delta S)^2 \text{ if } d_{(\tilde{n})} < 0,$$

where

C_L and C_O are constants

a is the sound speed

ρ_0 is reference density

V is relative volume

$\Delta S = \Delta S_1$ or ΔS_2 as discussed above

$$A_x = \frac{1}{\rho} \left(\frac{\partial \Sigma_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{T_{xy}}{y} \right)^* = \text{acceleration in x-direction}$$

$$A_y = \frac{1}{\rho} \left(\frac{\partial T_{xy}}{\partial x} + \frac{\partial \Sigma_{yy}}{\partial y} + \frac{\Sigma_{yy} - \Sigma_{\theta\theta}}{y} \right)^* = \text{acceleration in y-direction}$$

$$A = (A_x^2 + A_y^2)^{1/2}$$

$$n^1 = A_x/A$$

$$n^2 = A_y/A$$

$$\rho = \text{mass density}$$

CONCLUSION

The expression $d_{(\underline{n})}$ derived here is seen to be a measure of the rate of deformation of an element of length through a material point divided by that length in the direction \underline{n} . It was assumed that if \underline{n} were along the acceleration vector through the point and if $d_{(\underline{n})} < 0$ (compression), causing the grid established about that point to collapse so that the rear surface is overtaking the front surface, then a shock is forming. The validity of the "q" depends upon this assumption which seems to be the assumption made by von Neumann and Richtmyer and seems to be "physically reasonable." $d_{(\underline{n})}$ gives an exact measure of the tension or compression in the direction \underline{n} . The problem is to choose the "right" direction. The direction chosen (acceleration vector) is the one which indicates that particles are "bunching up" in the direction of impending motion, which is assumed to indicate the formation of a shock.

*These terms are set to zero for a plane problem.

APPENDIX A

THE MATERIAL DERIVATIVE OF ds^2

First we define the covariant partial derivative of a vector, which is indicated by the semicolon in the tensor expressions below*:

$$\begin{aligned} A^k_{;l} &\equiv \frac{\partial A^k}{\partial x^l} + \left\{ \begin{matrix} k \\ l m \end{matrix} \right\} A^m \\ A_{k;l} &\equiv \frac{\partial A_k}{\partial x^l} - \left\{ \begin{matrix} m \\ k l \end{matrix} \right\} A_m, \end{aligned} \quad (A.1)$$

where A^k is a contravariant vector and A_k is a covariant vector. The quantity

$$\left\{ \begin{matrix} k \\ l m \end{matrix} \right\} \equiv \frac{\partial^2 z^n}{\partial x^l \partial x^m} \frac{\partial x^k}{\partial z^n}$$

is the Christoffel symbol of the second kind. The quantities $A^k_{;l}$ and $A_{k;l}$ are second-order tensors. Next, we define the material or substantial derivative which is a time derivative with X^K held constant:

$$\frac{D}{Dt} (B^k_l) \equiv \frac{\partial B^k_l}{\partial t} + B^k_{l;m} \dot{x}^m \equiv \frac{\partial B^k_l}{\partial t} + B^k_{l;m} v^m \quad (A.2)$$

with $B^k_l = B^k_l(x^1, x^2, x^3, t)$, where $\dot{x}^m \equiv \partial x^m / \partial t \equiv Dx^m / Dt \equiv v^m$ is the velocity vector in the Eulerian system.

Now the quantity g_{kl} is a function of x^1, x^2, x^3 only and by Ricci's theorem:

$$g_{kl;m} \equiv 0,$$

hence:

$$\frac{D}{Dt} (g_{kl}) \equiv 0. \quad (A.3)$$

By considering the second of (A.1):

$$dx^k = x^k_{,K} dX^K \text{ at any time } t \quad (A.4)$$

where $x^k_{,K} \equiv \partial x^k / \partial X^K$ is called the displacement gradient.

*See Ref. 3, p. 439 ff.

Now, we calculate the material derivative of $x^k_{,K}$. First we recall that $x^k_{,K} = x^k_{,K}(X^1, X^2, X^3, t)$ but by the first of (A.1), $X^K = X^K(x^1, x^2, x^3, t)$ and hence we can consider:

$$x^k_{,K}(X^1, X^2, X^3, t) = a^k_K(x^1, x^2, x^3, t), \quad (\text{A.5})$$

then using (A.2) and (A.5):

$$\frac{D}{Dt} \left(x^k_{,K} \right) = \frac{D}{Dt} a^k_K(x^1, x^2, x^3, t) = \frac{\partial a^k_K}{\partial t} + a^k_{K;\ell} \dot{x}^\ell. \quad (\text{A.6})$$

Using (A.1) in (A.6):

$$\frac{D}{Dt} x^k_{,K} = \frac{\partial a^k_K}{\partial t} + \frac{\partial a^k_K}{\partial x^\ell} \dot{x}^\ell + \left\{ \begin{matrix} k \\ \ell m \end{matrix} \right\} a^m_K \dot{x}^\ell. \quad (\text{A.7})$$

Now the ordinary derivative with respect to time of a^k_K is given by:

$$\frac{d}{dt} \left(a^k_K \right) = \frac{\partial a^k_K}{\partial t} + \frac{\partial a^k_K}{\partial x^\ell} \dot{x}^\ell$$

and is as noted earlier $\dot{x}^\ell = v^\ell$, hence (A.7) becomes:

$$\frac{D}{Dt} x^k_{,K} = \frac{d}{dt} \left(a^k_K \right) + \left\{ \begin{matrix} k \\ \ell m \end{matrix} \right\} a^m_K v^\ell. \quad (\text{A.8})$$

If, now, we think of $a^k_K = x^k_{,K}(X^1, X^2, X^3, t)$ we can invert the order of differentiation in the first term on the right of (A.8) and write:

$$\frac{D}{Dt} x^k_{,K} = v^k_{,K} + \left\{ \begin{matrix} k \\ \ell m \end{matrix} \right\} v^\ell x^m_{,K}. \quad (\text{A.9})$$

By the chain rule of differentiation considering $v^k = v^k(x^1, x^2, x^3, t)$ and using the second of (A.1):

$$v^k_{,K} = v^k_{,m} x^m_{,K}$$

so that using (A.1):

$$\frac{D}{Dt} x^k_{,K} = \left(v^k_{,m} + \left\{ \begin{matrix} k \\ \ell m \end{matrix} \right\} v^\ell \right) x^m_{,K} = v^k_{;m} x^m_{,K}. \quad (\text{A.10})$$

Since D/Dt considers X^K constant, multiplying (A.10) by dX^K and using (A.4), yields:

$$\frac{D}{Dt} dx^k = v^k_{;\ell} dx^\ell. \quad (\text{A.11})$$

Now we are in a position to consider the material derivative of ds^2 .

Using (5):

$$\frac{D}{Dt} (ds^2) = \frac{D}{Dt} (g_{kl} dx^k dx^l) = g_{kl} \frac{D}{Dt} (dx^k) dx^l + g_{kl} dx^k \frac{D}{Dt} (dx^l)$$

where we used (A.3) to remove g_{kl} from inside the operator. If now (A.11) is used:

$$\frac{D}{Dt} (ds^2) = g_{kl} v^k_{;m} dx^m dx^l + g_{kl} v^l_{;m} dx^k dx^m. \quad (A.12)$$

As is well known the metric g_{kl} is a lowering operator,* i.e., $v_l = g_{lk} v^k$ and is symmetric. Using this and changing the dummy indices:

$$\frac{D}{Dt} (ds^2) = (v_{l;k} + v_{k;l}) dx^k dx^l = 2 d_{kl} dx^k dx^l \quad (A.13)$$

where $d_{kl} \equiv \frac{1}{2} (v_{k;l} + v_{l;k})$ is the symmetric part of the velocity gradient and is called the deformation rate tensor.

* See Ref. 3, p. 434.

APPENDIX B

EXPRESSIONS FOR $d_{(n)}$

We will now derive the expressions for $d_{(n)}$ in three orthogonal coordinate systems.

Before proceeding it is necessary to introduce the concept of physical components of a vector and a tensor.* In general, the components of a vector or a tensor do not have the same units. For a displacement vector with contravariant components referred to a cylindrical coordinates, as an example, we will show this.

Let:

$$\underline{u} = u^k \underline{g}_k \quad (B.1)$$

be the displacement vector. The base vector \underline{g}_k is defined by:

$$\underline{g}_k \equiv \frac{\partial \underline{p}}{\partial x^k} = \frac{\partial z^m}{\partial x^k} \underline{i}_m \quad (B.2)$$

where \underline{i}_m = unit vector along the rectangular coordinate axis z^m . In a cylindrical coordinate system $x^1 = r$, $x^2 = \theta$, $x^3 = z$ in the usual notation and $z^1 = x$, $z^2 = y$, $z^3 = z$ in the rectangular system in the usual notation so that:

$$z^1 = x^1 \cos x^2, \quad z^2 = x^1 \sin x^2, \quad z^3 = x^3$$

from which:

$$\left(\frac{\partial z^m}{\partial x^k} \right) = \begin{pmatrix} \cos x^2 & -x^1 \sin x^2 & 0 \\ \sin x^2 & x^1 \cos x^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$\begin{aligned} \underline{g}_1 &= (\cos x^2) \underline{i}_1 + (\sin x^2) \underline{i}_2 \\ \underline{g}_2 &= -(x^1 \sin x^2) \underline{i}_1 + (x^1 \cos x^2) \underline{i}_2 \\ \underline{g}_3 &= \underline{i}_3. \end{aligned}$$

Hence:

$$|\underline{g}_1| = 1, \quad |\underline{g}_2| = x^1, \quad |\underline{g}_3| = 1.$$

* See Ref. 3, p. 436 ff.

Now if \underline{u} is a displacement vector, it has the units of length L and since $|\underline{g}_1| = 1$ and $|\underline{g}_3| = 1$, u^1 and u^3 have units of length L but $|\underline{g}_2| = x^1$ has units L whence u^2 is unitless. Since $g_{k\ell} = \underline{g}_k \cdot \underline{g}_\ell$, we see that

$$|\underline{g}_k| = \sqrt{g_{\underline{k}\underline{k}}} \quad (\text{no sum on } k).^* \quad (\text{B.3})$$

In order to express the components of a vector in physical components, i.e., components that have the same units as the vector, it is necessary to take parallel projections of the vector on unit vectors along the coordinate curves. If we define such a unit vector:

$$\underline{e}_k = \underline{g}_k / \sqrt{g_{\underline{k}\underline{k}}} \quad (\text{B.4})$$

then we define the physical components of \underline{u} , denoted by $u^{(k)}$ by:

$$\underline{u} = u^{(k)} \underline{e}_k \quad (\text{B.5})$$

Since a vector is not dependent upon the coordinate axis used to measure it, we can write:

$$u^k \underline{g}_k = u^{(k)} \underline{e}_k$$

and using (B.4), we can write:

$$u^{(k)} = u^k \sqrt{g_{\underline{k}\underline{k}}} \quad , \quad u^k = u^{(k)} / \sqrt{g_{\underline{k}\underline{k}}} \quad (\text{B.6})$$

To obtain the physical components of the covariant components we lower the index, i.e.

$$u_k = g_{k\ell} u^\ell = \sum_{\ell} g_{k\ell} u^{(\ell)} / \sqrt{g_{\underline{\ell}\underline{\ell}}} \quad (\text{B.7})$$

To carry this definition to second-order tensors, a tensor B^k_{ℓ} is converted to a vector B^k by the use of a vector n^ℓ as follows:

$$B^k = B^k_{\ell} n^\ell \quad ,$$

then using (B.6) on B^k and n^ℓ one obtains:

$$B^{(k)}_{(\ell)} = B^k_{\ell} \sqrt{g_{\underline{k}\underline{k}} / g_{\underline{\ell}\underline{\ell}}} \quad (\text{B.8})$$

* It will be understood that where a pair of repeated indices are underlined, that no sum is to be taken.

Equation (B.8) gives the right physical components of B_{ℓ}^k . The left physical components are given by:

$$B_{(\ell)}^{(k)} = B_{\ell}^k \sqrt{g_{kk}/g_{\ell\ell}}. \quad (\text{B.9})$$

In general, $B_{(\ell)}^{(k)} \neq B_{(\ell)}^{(k)}$. Now:

$$d_{(\tilde{n})} = d_{k\ell} n^k n^{\ell} = n_k d_{\ell}^k n^{\ell}$$

using (B.6-B.8):

$$d_{(\tilde{n})} = \left(\sum_m g_{km} \frac{n^{(m)}}{\sqrt{g_{mm}}} \right) \left(d_{(\ell)}^{(k)} \sqrt{\frac{g_{\ell\ell}}{g_{kk}}} \right) \left(\frac{n^{(\ell)}}{\sqrt{g_{\ell\ell}}} \right)$$

or

$$d_{(\tilde{n})} = \sum_k \sum_{\ell} \sum_m \frac{g_{km}}{\sqrt{g_{mm} g_{kk}}} n^{(m)} d_{(\ell)}^{(k)} n^{(\ell)}.$$

For an orthogonal coordinate system $g_{km} = 0$ for $k \neq m$, whence:

$$d_{(\tilde{n})} = \sum_k \sum_{\ell} n^{(k)} d_{(\ell)}^{(k)} n^{(\ell)}, \quad (\text{B.10})$$

and writing (B.10) in component form:

$$\begin{aligned} d_{(\tilde{n})} = & d_{(1)}^{(1)} [n^{(1)}]^2 + d_{(2)}^{(2)} [n^{(2)}]^2 + d_{(3)}^{(3)} [n^{(3)}]^2 \\ & + d_{(2)}^{(1)} n^{(1)} n^{(2)} + d_{(1)}^{(2)} n^{(1)} n^{(2)} + d_{(3)}^{(1)} n^{(1)} n^{(3)} \\ & + d_{(1)}^{(3)} n^{(1)} n^{(3)} + d_{(3)}^{(2)} n^{(2)} n^{(3)} + d_{(2)}^{(3)} n^{(2)} n^{(3)}. \end{aligned} \quad (\text{B.11})$$

We have defined:

$$d_{k\ell} = \frac{1}{2} (v_{k;\ell} + v_{\ell;k}),$$

and we obtain from this:

$$d_{\ell}^k = g^{km} d_{m\ell} = \frac{1}{2} (v_{;\ell}^k + g^{km} v_{\ell;m}),$$

where g^{km} is the metric tensor for the reciprocal base vectors and its matrix is given by:

$$(g^{km}) = (g_{km})^{-1}.$$

Now

$$v_{\ell;m} = g_{\ell n} v_{;m}^n$$

so that

$$d_{\ell}^k = \frac{1}{2} \left(v_{;\ell}^k + g_{\ell n} v_{;m}^n g^{mk} \right). \quad (B.12)$$

The matrix for d_{ℓ}^k can thus be obtained from:

$$\left(d_{\ell}^k \right) = \frac{1}{2} \left\{ \left(v_{;\ell}^k \right) + \left(g_{\ell n} v_{;m}^n g^{mk} \right)^T \right\}, \quad (B.13)$$

where $(A_n^m)^T$ indicates the transpose of the matrix (A_n^m) .

For an orthogonal coordinate system:

$$(g_{\ell n}) = \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix}, \quad (g^{mk}) = \begin{pmatrix} 1/g_{11} & 0 & 0 \\ 0 & 1/g_{22} & 0 \\ 0 & 0 & 1/g_{33} \end{pmatrix},$$

using these in (B.13) and (B.8) we can write the matrix of d_{ℓ}^k in physical components as:

$$\left(d_{\ell}^{(k)} \right) = \begin{pmatrix} v_{;1}^1 & \frac{1}{2} \left[\sqrt{\frac{g_{11}}{g_{22}}} v_{;2}^1 + \sqrt{\frac{g_{22}}{g_{11}}} v_{;1}^2 \right] & \frac{1}{2} \left[\sqrt{\frac{g_{11}}{g_{33}}} v_{;3}^1 + \sqrt{\frac{g_{33}}{g_{11}}} v_{;1}^3 \right] \\ \frac{1}{2} \left[\sqrt{\frac{g_{22}}{g_{11}}} v_{;1}^2 + \sqrt{\frac{g_{11}}{g_{22}}} v_{;2}^1 \right] & v_{;2}^2 & \frac{1}{2} \left[\sqrt{\frac{g_{22}}{g_{33}}} v_{;3}^2 + \sqrt{\frac{g_{33}}{g_{22}}} v_{;2}^3 \right] \\ \frac{1}{2} \left[\sqrt{\frac{g_{33}}{g_{11}}} v_{;1}^3 + \sqrt{\frac{g_{11}}{g_{33}}} v_{;3}^1 \right] & \frac{1}{2} \left[\sqrt{\frac{g_{33}}{g_{22}}} v_{;2}^3 + \sqrt{\frac{g_{22}}{g_{33}}} v_{;3}^2 \right] & v_{;3}^3 \end{pmatrix}$$

Using (B. 6)

$$(n^{(k)}) = \left(n^1 \sqrt{g_{11}} \quad n^2 \sqrt{g_{22}} \quad n^3 \sqrt{g_{33}} \right).$$

Putting these last two in (B.11):

$$\begin{aligned} d_{(n)} = & v_{;1}^1 (n^1)^2 g_{11} + v_{;2}^2 (n^2)^2 g_{22} + v_{;3}^3 (n^3)^2 g_{33} + \left(g_{22} v_{;1}^2 + g_{11} v_{;2}^1 \right) n^1 n^2 \\ & + \left(g_{11} v_{;3}^1 + g_{33} v_{;1}^3 \right) n^1 n^3 + \left(g_{33} v_{;2}^3 + g_{22} v_{;3}^2 \right) n^2 n^3. \quad (B.14) \end{aligned}$$

Since we desire $d_{(\underline{n})}$ in the direction of acceleration, we will express \underline{n} as follows:

$$\underline{n} = \left(\frac{\sqrt{g_{11}} A^1}{|\underline{A}|} \quad \frac{\sqrt{g_{22}} A^2}{|\underline{A}|} \quad \frac{\sqrt{g_{33}} A^3}{|\underline{A}|} \right)$$

where

$$|\underline{A}| = \sqrt{g_{11}(A^1)^2 + g_{22}(A^2)^2 + g_{33}(A^3)^2} \equiv \text{acceleration,}$$

then we may write (B.14) as:

$$d_{(\underline{a})} = \frac{v_{;1}^1 (A^1)^2 g_{11} + v_{;2}^2 (A^2)^2 g_{22} + v_{;3}^3 (A^3)^2 g_{33} + (g_{22} v_{;1}^2 + g_{11} v_{;2}^1) A^1 A^2}{g_{11}(A^1)^2 + g_{22}(A^2)^2 + g_{33}(A^3)^2} + \frac{(g_{11} v_{;3}^1 + g_{33} v_{;1}^3) A^1 A^3 + (g_{22} v_{;3}^2 + g_{33} v_{;2}^3) A^2 A^3}{g_{11}(A^1)^2 + g_{22}(A^2)^2 + g_{33}(A^3)^2} \quad (\text{B.15})$$

For a rectangular coordinate system:

$$\begin{aligned} x^1 &= x, \quad x^2 = y, \quad x^3 = z \\ g_{11} &= g_{22} = g_{33} = 1 \\ v_{;j}^i &= \partial \dot{x}^i / \partial x^j \end{aligned}$$

For a cylindrical coordinate system:

$$\begin{aligned} x^1 &= r, \quad x^2 = \theta, \quad x^3 = z \\ g_{11} &= g_{33} = 1, \quad g_{22} = r^2 \\ v_{;j}^i &= \begin{pmatrix} \frac{\partial \dot{r}}{\partial r} & \frac{\partial \dot{r}}{\partial \theta} - r \dot{\theta} & \frac{\partial \dot{r}}{\partial z} \\ \frac{\partial \dot{\theta}}{\partial r} + \frac{\dot{\theta}}{r} & \frac{\partial \dot{\theta}}{\partial \theta} + \frac{\dot{r}}{r} & \frac{\partial \dot{\theta}}{\partial z} \\ \frac{\partial \dot{z}}{\partial r} & \frac{\partial \dot{z}}{\partial \theta} & \frac{\partial \dot{z}}{\partial z} \end{pmatrix} \end{aligned}$$

For a spherical coordinate system:

$$\begin{aligned} x^1 &= r, \quad x^2 = \theta, \quad x^3 = \psi \\ g_{11} &= 1, \quad g_{22} = r^2, \quad g_{33} = r^2 \sin^2 \theta \end{aligned}$$

$$(v_{ij}^i) = \begin{pmatrix} \frac{\partial \dot{r}}{\partial r} & \frac{\partial \dot{r}}{\partial \theta} - r\dot{\theta} & \frac{\partial \dot{r}}{\partial \psi} - r\dot{\psi} \sin^2 \theta \\ \frac{\partial \dot{\theta}}{\partial r} + \frac{\dot{\theta}}{r} & \frac{\partial \dot{\theta}}{\partial \theta} + \frac{\dot{r}}{r} & \frac{\partial \dot{\theta}}{\partial \psi} - \dot{\psi} \sin \theta \cos \theta \\ \frac{\partial \dot{\psi}}{\partial r} + \frac{\dot{\psi}}{r} & \frac{\partial \dot{\psi}}{\partial \theta} + \dot{\psi} \cot \theta & \frac{\partial \dot{\psi}}{\partial \psi} + \frac{\dot{r}}{r} + \dot{\theta} \cot \theta \end{pmatrix}$$

Using these in (B.15) we can write:

For a rectangular coordinate system in three dimensions:

$$d_{(\underline{A})} = \frac{\frac{\partial \dot{x}}{\partial x} (A_x)^2 + \frac{\partial \dot{y}}{\partial y} (A_y)^2 + \frac{\partial \dot{z}}{\partial z} (A_z)^2 + \left(\frac{\partial \dot{x}}{\partial y} + \frac{\partial \dot{y}}{\partial x} \right) A_x A_y + \left(\frac{\partial \dot{x}}{\partial z} + \frac{\partial \dot{z}}{\partial x} \right) A_x A_z + \left(\frac{\partial \dot{y}}{\partial z} + \frac{\partial \dot{z}}{\partial y} \right) A_y A_z}{(A_x)^2 + (A_y)^2 + (A_z)^2}$$

For a cylindrical coordinate system:

$$d_{(\underline{A})} = \frac{\frac{\partial \dot{r}}{\partial r} (A_r)^2 + \left(\frac{\partial \dot{\theta}}{\partial \theta} + \frac{\dot{r}}{r} \right) (rA_\theta)^2 + \frac{\partial \dot{z}}{\partial z} (A_z)^2 + \left(\frac{\partial \dot{r}}{\partial \theta} + r^2 \frac{\partial \dot{\theta}}{\partial r} \right) A_r A_\theta}{(A_r)^2 + (rA_\theta)^2 + (A_z)^2} + \frac{\left(\frac{\partial \dot{r}}{\partial z} + \frac{\partial \dot{z}}{\partial r} \right) A_r A_z + \left(\frac{\partial \dot{\theta}}{\partial z} + r^2 \frac{\partial \dot{\theta}}{\partial z} \right) A_\theta A_z}{(A_r)^2 + (rA_\theta)^2 + (A_z)^2}$$

For a spherical coordinate system:

$$d_{(\underline{A})} = \frac{\frac{\partial \dot{r}}{\partial r} (A_r)^2 + \left(\frac{\partial \dot{\theta}}{\partial \theta} + \frac{\dot{r}}{r} \right) (rA_\theta)^2 + \left(\frac{\partial \dot{\psi}}{\partial \psi} + \frac{\dot{r}}{r} + \dot{\psi} \cot \theta \right) (rA_\psi \sin \theta)^2}{(A_r)^2 + (rA_\theta)^2 + (rA_\psi \sin \theta)^2} + \frac{\left(\frac{\partial \dot{r}}{\partial \theta} + r^2 \frac{\partial \dot{\theta}}{\partial r} \right) A_r A_\theta + \left(\frac{\partial \dot{r}}{\partial \psi} + r^2 \sin^2 \theta \frac{\partial \dot{\psi}}{\partial r} \right) A_r A_\psi + \left(\frac{\partial \dot{\theta}}{\partial \psi} + \sin^2 \theta \frac{\partial \dot{\psi}}{\partial \theta} \right) r^2 A_\theta A_\psi}{(A_r)^2 + (rA_\theta)^2 + (rA_\psi \sin \theta)^2}$$

It is easily seen from the above that for a one-dimensional system:

$$d_{(\underline{A})} = \frac{\partial \dot{x}}{\partial x}$$

which is the quantity used by von Neumann to activate his "q" and whose magnitude was used in forming the "q."

It will be noted that any direction could be selected for \underline{n} and in case some other direction is desired, (B.14) can be used to calculate $d_{(\underline{n})}$.

Quite obviously the first two expressions above for $d_{(\underline{A})}$ can be written as:

$$d_{(\underline{A})} = \frac{\frac{\partial \dot{x}}{\partial x} (A_x)^2 + \frac{\partial \dot{y}}{\partial y} (A_y)^2 + \left(\frac{\partial \dot{x}}{\partial y} + \frac{\partial \dot{y}}{\partial x} \right) A_x A_y}{(A_x)^2 + (A_y)^2}$$

if cylindrical symmetry is assumed with no angular motion and y is either the radial direction or the other rectangular direction. In this case the components of the acceleration vector are obtained from the motion equations as given in Ref. 2, p. 20 and are reproduced below:

$$A_x = \frac{1}{\rho} \left(\frac{\partial \Sigma_{xx}}{\partial x} + \frac{\partial T_{xy}}{\partial y} + \frac{T_{xy}}{y} \right)^* = \text{acceleration in x-direction}$$

$$A_y = \frac{1}{\rho} \left(\frac{\partial T_{xy}}{\partial x} + \frac{\partial \Sigma_{yy}}{\partial y} + \frac{\Sigma_{yy} - \Sigma_{\theta\theta}}{y} \right)^* = \text{acceleration in y-direction}$$

where

Σ_{ii} = normal stress in i direction

T_{ij} ($i \neq j$) = shear stress in the j direction on a plane with a normal in the direction i

ρ = mass density.

In connection with the HEMP code (see Ref. 2) the expression $d_{(\underline{n})}$ has another application. This is in connection with the problem involving a material with a different yield strength in compression than it has in tension. In such a case one must be able to determine whether there is compression or tension in the direction of motion. The quantity $d_{(\underline{n})}$ can answer this if \underline{n} is along the velocity vector.

* These terms are set to zero for the plane case.

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